

Can Disorder Induce a Finite Thermal Conductivity in 1D Lattices?

Baowen Li,^{1,2,*} Hong Zhao,^{2,3} and Bambi Hu^{2,4}

¹*Department of Physics, National University of Singapore, 119260 Singapore*

²*Department of Physics and Center for Nonlinear Studies, Hong Kong Baptist University, Hong Kong, China*

³*Department of Physics, Lanzhou University, 730000 Lanzhou, China*

⁴*Department of Physics, University of Houston, Houston, Texas 77204-506*

(Received 2 November 1999)

We study heat conduction in one-dimensional mass-disordered harmonic and anharmonic lattices. It is found that the thermal conductivity κ of the disordered anharmonic lattice is finite at low temperature, whereas it diverges as $\kappa \sim N^{0.43}$ at high temperature. Moreover, we demonstrate that a unique nonequilibrium stationary state in the disordered harmonic lattice does not exist at all.

DOI: 10.1103/PhysRevLett.86.63

PACS numbers: 44.10.+i, 05.70.Ln, 05.45.-a, 66.70.+f

Can disorder induce a finite thermal conductivity in one dimensional (1D) lattices? This question arose immediately after Anderson's finding of localization [1]. It has been commonly believed that disorder scatters normal modes and induces a diffusive energy transport that leads to a normal heat conduction. However, the early numerical as well as theoretical studies show that the thermal conductivity in 1D (mass) disordered harmonic lattice is proportional to $N^{1/2}$, where N is the length of the lattice [2–4]. The reason for this divergent thermal conductivity has not been clear up to now. In fact, the existing theories [3,4] do not prove that a unique nonequilibrium stationary state could be reached in a disordered harmonic lattice. Intending to obtain a finite thermal conductivity, Payton *et al.* [2] tried to add an anharmonicity to the disordered lattice. It was found that the anharmonicity did enhance the heat current, but Payton *et al.* were not able to verify the validity of the Fourier law in such systems due to limited computer facility. Therefore, whether disorder can induce a finite thermal conductivity is still a puzzle.

In the past three decades, many works have been devoted to seeking such a model whose heat conduction behavior obeys the Fourier law, i.e., $J = -\kappa dT/dx$. The primary motivation is to find out whether it is possible to prove or disprove a given 1D many-body Hamiltonian system having or not having a finite thermal conductivity. If it is possible, then how can one calculate transport coefficients from microscopic Hamiltonian. The emergence of chaos in past years sheds some light on this old but rather fundamental problem. It stimulated further study of heat conduction in nonintegrable systems, with attempts to find the dynamical origin of the thermodynamical properties, such as irreversibility, etc. [5]. For this purpose, a wide range of nonintegrable systems, such as the Lorenz gas model [6], the “ding-a-ling” and “alike” models [7], the Fermi-Pasta-Ulam (FPU) model [8], the Frenkel-Kontorova model [9], the diatomic Toda lattice [10], the Heisenberg spin lattice [11], the ϕ^4 lattice [12], and the sinh-Gordon and bounded single-well models [13], etc., has been invoked. Most recently, the study has been extended to systems having periodic interparticle potential

[14]. However, as we have already pointed out [12], nonintegrability is only a *necessary* condition for the formation of a temperature gradient but *not a sufficient* one for a finite thermal conductivity.

A rigorous proof of the necessary and sufficient condition for the Fourier law is still lacking, even though some progress in this direction has been achieved [15]. Facing such a situation, we have to rely on large scale molecular dynamics simulations to obtain a deep insight of the underlying mechanism of the divergent and/or finite thermal conductivity. Recently [12], in searching for the underlying mechanism of the energy transport, we found that the (mass) uniform lattice systems can be classified into three categories: integrable one, nonintegrable one with on-site potential, and nonintegrable one without on-site potential. We discovered that the on-site potential plays a very important role. It destroys the momentum conservation, produces a diffusive energy transport, and thus leads to a finite thermal conductivity. In nonintegrable lattices without on-site potential, the scattering of solitary waves is found to be responsible for the divergent thermal conductivity $\kappa \sim N^{0.43}$ in the FPU and alike models.

In this Letter, we study the effect of disorder on heat conduction in 1D lattices. The Hamiltonian of the models we are considering can be written as

$$H = \sum_i H_i, \quad H_i = \frac{p_i^2}{2m_i} + V(x_{i-1}, x_i), \quad (1)$$

where $V(x_{i-1}, x_i)$ stands for the interaction potential of the nearest-neighbor particles. In our study the mass of particles is given by

$$m_i = m_0 + \lambda(R_i - 0.5), \quad (2)$$

where λ is a parameter adjusting the amplitude of the random mass, and R_i is a random number distributed uniformly in the interval of (0, 1).

Disordered anharmonic lattices.—In this case the interparticle potential takes the form of that in the FPU model,

$$V(x_{i-1}, x_i) = \frac{1}{2} (x_i - x_{i-1})^2 + \frac{\beta}{4} (x_i - x_{i-1})^4. \quad (3)$$

$\beta = 1$ throughout this paper except otherwise stated. We call the model the disordered FPU (DFPU) model. In our numerical simulations the Nosé-Hoover thermostats [16] were put on the first and the last particles, keeping them at temperatures T_+ and T_- , respectively. The eighth-order Runge-Kutta algorithm was used to solve the coupled differential equations. All computations were carried out in double precision. Usually the stationary state set in after 10^6 – 10^7 time units; thereafter the time average $\langle J_i \rangle$ ($J_i = \dot{x}_i \partial V / \partial x_{i+1}$) was found to be site independent, and thus is denoted by J .

In Fig. 1(a), we present JN versus N for the FPU and the DFPU models with $T_+ = 3$ and $T_- = 2$. Both models have a similar (almost indistinguishable) temperature profile [Fig. 1(b)]. In both cases, the temperature gradient is proportional to N^{-1} ; thus $JN \propto \kappa$. Best fitting in Fig. 1(a) yields $\kappa \sim N^{0.43 \pm 0.01}$. This implies that in both models the thermal conductivity diverges in the same way. More numerics show that in this high temperature regime, the disorder does not help converge the thermal conductivity; it only decreases the value of heat current.

Interesting things turn out when the temperature of the thermostats is decreased. In Fig. 1(c), JN versus N is plotted for the DFPU model at three different values of disorder $\lambda = 0.2, 0.3$, and 0.4 , respectively, with $T_+ = 10^{-3}$ and $T_- = 5 \times 10^{-4}$. When $N < N_c$, JN increases monotonically with N . When $N > N_c$, JN saturates; namely, κ becomes an N -independent constant. This result indicates that the heat conduction obeys Fourier law when the size of the 1D lattice becomes larger than N_c . However, in this temperature regime, the FPU model and the harmonic lattice have the same heat conduction behavior [12]. This is reflected in the temperature profile shown in Fig. 1(d). It

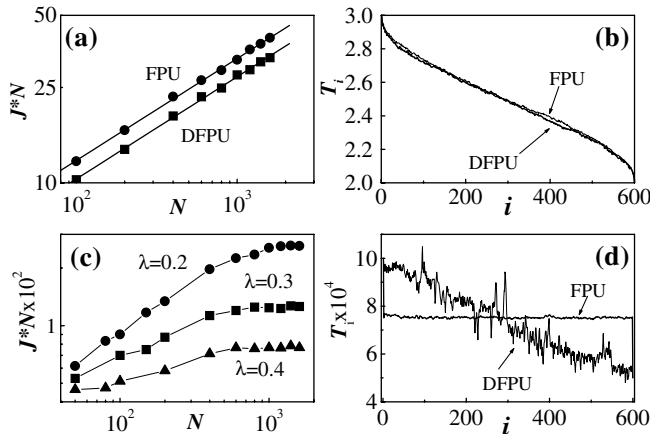


FIG. 1. JN versus N (a) and temperature profiles (b) for DFPU model ($\lambda = 0.4$) and the FPU model at high temperature, $T_+ = 3$ and $T_- = 2$. The solid lines in (a) are the best fitting ones; both have the same slope, $\alpha = 0.43 \pm 0.01$. (c) JN versus N for the DFPU model with different values of disorder at low temperature, $T_+ = 10^{-3}$ and $T_- = 5 \times 10^{-4}$. The lines are drawn to guide the eye. (d) Same as (b) but for the case of low temperature.

demonstrates that no temperature gradient can be formed, and the stationary state corresponds to $T = (T_+ + T_-)/2$.

In Fig. 2, we show $J(N)/J(2N)$ versus $T = (T_+ + T_-)/2$ for the FPU (solid triangle) and the DFPU (solid circle) models, where $J(N)$ is the heat current for the lattice of length N . The transition of the FPU model to a harmonic lattice happens when the temperature is decreased below a threshold value of T_c ($\approx 10^{-2}$). This is illustrated in Fig. 2 by an abrupt decrease of $J(N)/J(2N)$ from 1.5 to 1. On the other hand, within almost the same temperature range the heat conduction in the DFPU model undergoes another transition. This transition is demonstrated by an abrupt increase of $J(N)/J(2N)$ from about 1.5 to 2 when $T < T_c$. This implies that the DFPU model transforms from an abnormal thermal conductor to a normal one.

The above results of the FPU model can be understood from the scattering mechanism of solitary waves. As we discovered [12], the scattering between solitary waves from opposite directions causes an energy loss that gives rise to a temperature gradient. However, the momentum conservation in the FPU model prohibits a diffusive energy transport. The interaction of the solitary waves depends on the initial excitation. When $T < T_c$, the solitary waves cannot be excited any more, and the energy is transported by linear excitations—phonons. Thus the FPU model behaves like a harmonic one.

In order to clarify the underlying mechanism of the heat conduction in the disordered model, we study the dynamics of a single excitation. Figure 3(a) shows a snapshot of energy density H_i in a DFPU lattice at $t = 200$ for an initial excitation on the left end, i.e., $p_1 = 3, p_i = 0$, for $i \neq 1$. A solitary wave is excited and propagates to $i = 250$. If we decrease the energy of initial excitation below

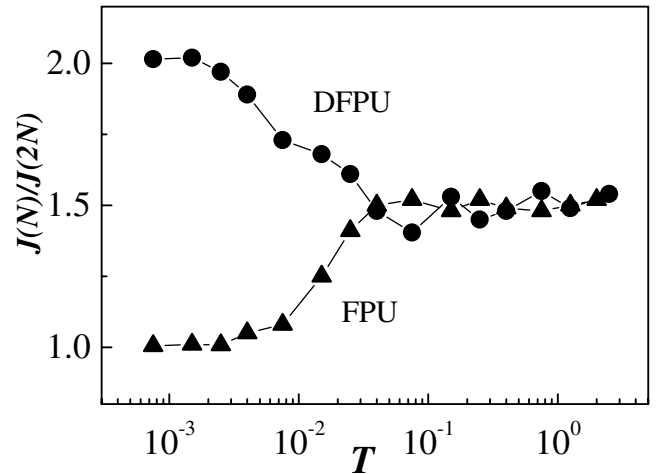


FIG. 2. $J(N)/J(2N)$ (for $N = 600$) versus the average temperature $T = (T_+ + T_-)/2$ in the semilogarithmic scale for the DFPU (solid circle) ($\lambda = 0.4$) and the FPU (solid triangle) models. The FPU model shows a transition to a harmonic lattice with the decrease of the temperature. However, the DFPU model changes from a divergent thermal conductor to a normal one as the temperature is decreased.

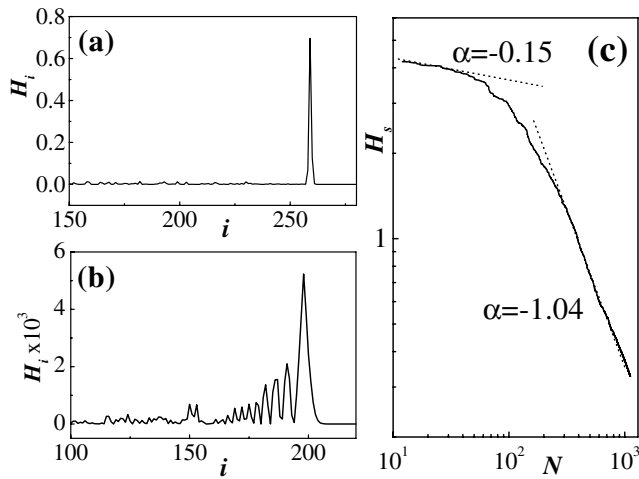


FIG. 3. Energy distribution in space at time $t = 200$ for high-excitation solitary waves (a) and low-excitation phonons (b) for a DFPU lattice with disorder $\lambda = 0.4$. (c) The energy of solitary waves on different sites. The dotted lines are the best fitting ones with the data in initial stage and in final stage, respectively. The different slopes (given in the figure) show that the energy decays at a different rate for solitary waves (initial stage) and phonons (final stage).

a threshold value, we find that the energy is no longer localized, namely, the solitary wave disappears. Instead, a traveling wave packet, linear excitations, is created and moves diffusively [see Fig. 3(b)]. However, unlike in the case of the FPU model, when a single solitary wave or a linear wave packet travels along the disordered lattice, its energy will decrease due to the scattering from the disorder. An interesting phenomenon is that solitary waves and phonons obey different scattering laws, as is shown in Fig. 3(c). In this figure we plot the energy versus the distance of the solitary wave excited in Fig. 3(a). We see that both in initial and final stages, the energy decays in power law $H_s \sim N^{-\alpha}$ but with different exponents, $\alpha \approx 0.15$ in the initial stage and $\alpha \approx 1$ in the final stage. The former represents the scattering of solitary waves by disorder, and the latter represents the scattering of phonons by disorder as in the final stage when the energy becomes so low that the solitary waves cannot be excited any more.

With the above picture, we can explain the numerical results of the DFPU model shown in Figs. 1 and 2. At high temperature [Figs. 1(a), 1(b), and 2], energy is transported mainly by solitary waves which encounter two kinds of scattering: scattering from solitary waves and scattering from disorder. The scaling law of energy loss caused by the two scattering are $N^{-\alpha}$ but with different values of α , $\alpha \approx 0.5$ for the former [12] and $\alpha \approx 0.15$ for the latter [see Fig. 3(c)]. In the thermodynamic limit the main cause of energy loss comes from the scattering of solitary waves. Thus at high temperature the DFPU model shows the same scaling law as the FPU model as is shown in Fig. 1(a). In this case the disorder cannot induce a finite thermal conductivity, but it decreases the total heat current only.

The situation becomes different at low temperature [Figs. 1(c), 1(d), and 2]. In this case, the solitary wave is hardly excited. The energy is transported by phonons. The scattering of phonons by disorder becomes a dominant factor for energy loss. Thus the energy decays as N^{-1} as is shown in Fig. 3(c), which implies a finite thermal conductivity. This prediction is confirmed by a direct calculation of JN given in Fig. 1(c). It is natural to relate the saturation phenomenon of JN in Fig. 1(c) to the localization of phonons in the system, wherein the localization length l is an important scale. If the length of the lattice N is shorter than l , the thermal conductivity is expected to be divergent. On the contrary, if the lattice is much longer than l , then a normal heat conduction could be realized. This is indeed the case shown in Fig. 1(c). The threshold value N_c is approximately 500, 700, and 1000 for the three different values of the disorder $\lambda = 0.4, 0.3$, and 0.2 , respectively. Extensive numerical simulations confirm that $N_c \propto 1/\lambda$. This is of order l , because $l \propto \langle m \rangle / \sqrt{\langle (m - \langle m \rangle)^2 \rangle} \sim 1/\lambda$ [4].

Disordered harmonic lattices.—It was shown theoretically [3,4] that the thermal conductivity diverges as $\kappa \sim N^{1/2}$ in 1D disordered harmonic lattice [$\beta = 0$ in Eq. (3)]. The proof was based on an assumption that a unique nonequilibrium stationary state could be reached in such systems. However, to the best of our knowledge, this assumption has not been verified numerically. This motivated us to do further investigation.

We find that a stationary state, with erratic temperature fluctuation, can be set up as is shown in Fig. 4(a). The states starting from the same initial condition ($T^0 = 0.01$) are almost indistinguishable at different times $t = 10^6$ and $t = 10^7$. (Please note the inset for magnification.) This guarantees the existence of the stationary state. Unfortunately, such a state depends sensitively on the initial condition. In the same figure, we show another stationary state (dashed line) formed from a different initial condition $T^0 = 3$. It differs greatly from that one of $T^0 = 0.01$. This result means that the nonequilibrium stationary state in the disordered harmonic lattice is *not unique*.

To obtain a clear picture, we turn to a simple model, a lattice that consists of only two types of atoms, one with mass $m = 1$ the other with mass $m = 0.5$. A segment of light atoms is embedded in the middle of the other two segments of heavy atoms. Two ends of the lattice are put in the thermostats with the same temperature $T_+ = T_- = 4$. Two stationary states from two different initial conditions $T^0 = 0.1$ and $T^0 = 1$ are shown in Fig. 4(b). Again, no unique stationary state can be formed. However, adding a small fraction of anharmonicity, $\beta = 10^{-8}$, to this lattice produces a completely different picture. With this tiny anharmonicity, we can obtain not only a smooth temperature profile but also a unique stationary state; see Fig. 4(b).

The above results show that although the anharmonicity alone is not enough to yield a finite thermal conductivity, it

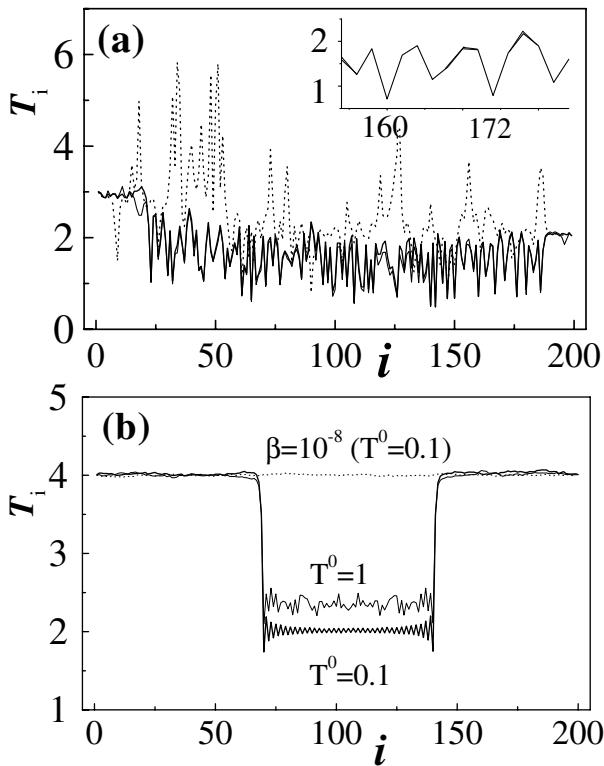


FIG. 4. (a) Temperature distribution of a disordered harmonic lattice ($\lambda = 1$) from different initial conditions, the solid lines for $T^0 = 0.01$ at 10^6 and 10^7 time units (see also the inset for the magnification of a small interval), respectively, and the dotted line for $T^0 = 3$ at 10^7 time units. (b) The temperature profile (solid line) of a harmonic lattice consists of three uniform segments. The left and the right segments are atoms of the mass $m = 1$ while the middle one consists of atoms of mass $m = 0.5$. $T_+ = T_- = 4$. The dashed line is for the same system but with anharmonicity $\beta = 10^{-8}$.

plays a crucial role in establishing a unique nonequilibrium stationary state in disordered lattices.

In summary, we have studied heat conduction in 1D disordered harmonic and anharmonic lattices. Our numerical results show that at low temperature disorder can induce a finite thermal conductivity. The magnitude of the disorder does not affect the results in the thermodynamical limit. It only determines the localization length and threshold length of a lattice having a finite thermal conductivity. However, at high temperature, the disordered anharmonic lattice shows a divergent thermal conductivity, which is similar to that of the FPU model. In addition, we provide

numerical evidence showing that the nonequilibrium stationary state in a disordered harmonic lattice is *not unique*.

B. L. was supported in part by Academic Research Fund of National University of Singapore. This work was also supported in part by Hong Kong Research Grant Council and the Hong Kong Baptist University Faculty Research Grant.

*Author to whom correspondence should be addressed.

Email address: phylbw@nus.edu.sg

- [1] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
- [2] D. N. Payton III and W. M. Visscher, Phys. Rev. **156**, 1032 (1967); D. N. Payton III, M. Rich, and W. M. Visscher, *ibid.* **160**, 706 (1967).
- [3] Z. Rieder, J. L. Lebowitz, and E. Lieb, J. Math. Phys. (N.Y.) **8**, 1073 (1967); A. Casher and J. L. Lebowitz, *ibid.* **8**, 1701 (1971); A. J. O'Connor and J. L. Lebowitz, *ibid.* **15**, 692 (1974).
- [4] H. Matsuda and K. Ishii, Suppl. Prog. Theor. Phys. **45**, 56 (1970).
- [5] *Focus issue: Chaos and Irreversibility* [Chaos **8** (1998)]; J. Lebowitz, Physica (Amsterdam) **263A**, 516 (1999); I. Prigogine, *ibid.* **263**, 528 (1999); D. Ruelle, *ibid.* **263**, 540 (1999).
- [6] J. L. Lebowitz and H. Spohn, J. Stat. Phys. **19**, 633 (1978); D. Alonso, R. Artuso, G. Casati, and I. Guarneri, Phys. Rev. Lett. **82**, 1859 (1999).
- [7] G. Casati, J. Ford, F. Vivaldi, and W. M. Visscher, Phys. Rev. Lett. **52**, 1861 (1984); T. Prosen and M. Robnik, J. Phys. A **25**, 3449 (1992); D. J. R. Mimmagh and L. E. Ballentine, Phys. Rev. E **56**, 5332 (1997); H. A. Posch and Wm. G. Hoover, *ibid.* **58**, 4344 (1998).
- [8] H. Kaburaki and M. Machida, Phys. Lett. A **181**, 85 (1993); S. Lepri, R. Livi, and A. Politi, Phys. Rev. Lett. **78**, 1896 (1997); A. Fillipov, B. Hu, B. Li, and A. Zeltser, J. Phys. A **31**, 7719 (1998).
- [9] B. Hu, B. Li, and H. Zhao, Phys. Rev. E **57**, 2992 (1998).
- [10] T. Hatano, Phys. Rev. E **59**, R1 (1999).
- [11] A. Dhar and D. Dhar, Phys. Rev. Lett. **82**, 480 (1999).
- [12] B. Hu, B. Li, and H. Zhao, Phys. Rev. E **61**, 3828 (2000).
- [13] G. P. Tsironis, A. R. Bishop, A. V. Savin, and A. V. Zolotaryuk, Phys. Rev. E **60**, 6610 (1999).
- [14] C. Giardin'a, R. Livi, A. Politi, and M. Vassalli, Phys. Rev. Lett. **84**, 2144 (2000); O. V. Gendelman and A. V. Savin, *ibid.* **84**, 2381 (2000).
- [15] T. Prosen and D. K. Campbell, Phys. Rev. Lett. **84**, 2857 (2000).
- [16] S. Nosé, J. Chem. Phys. **81**, 511 (1984); W. G. Hoover, Phys. Rev. A **31**, 1695 (1985).